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Abstract

As one necessary step for a good modeling, this study was aimed at analyzing the sensitivity of GreenLab model for maize. When instantaneous value of biomass generation is considered as the output, the system tends to be linear, the level is above 94% in SRC(Standardized Regression coefficients)study. Conversion efficiency and characteristic surface are proved to be the most sensitive factors. In Sobol's measure, we excluded the two most sensitive factors in the analysis, then the system linearity tends to be weaker and we got the detailed sensitivity indexes for the other uncertain parameters, by which we get the clearer driven force of maize growth in different stages.

1. Introduction

Modeling represents a necessary tool for understanding plant growth and developing predictive tools for decision making. Good modeling practice requires that the modeler provides an evaluation of the confidence in the model. Sensitivity analysis (SA) is the study of how the variation (uncertainty) in the output of a mathematical model can be apportioned, qualitatively or quantitatively, to different sources of variation in the input factors of a model [1].

So sensitivity Analysis (SA) has role of ordering by importance the strength and relevance of the inputs in determining the variations of the output variables of interest. Such information may provide some help for model assessment: SA can help the modeler to measure model adequacy (e.g.does the model fit observation) and relevance (e.g. is the model-based inference robust), to identify critical regions in the inputs space (e.g. which combination of factors corresponds to the highest risk), to detect interactions between factors, to establish priorities for research and experimentations and to simplify model structure [2].

If sensitivity analysis is quite usual in crop and plant growth models, it had long been restricted to local sensitivity analysis or to analysis of variance for linear models. An interesting exception is given by [3], for a variance-based analysis for the crop model STICS, with the objective of choosing the main parameters to be estimated. The analysis is first made module by module and then sensitivities of each module are compared for overall model outputs. The main factors addressed concern the interaction with the environment, which is of crucial interest.

Our objective in this paper is to study the interest of global sensitivity analysis and its last developments for the GreenLab model (see [4], [5], [6]), and more generally for a better understanding of source-sink dynamics and internal driving forces during plant growth. Potentially, this work should result in a better parameterization of the GreenLab model. As detailed by [7], there are two groups of parameters in the model: the observed ones, that can be directly obtained by experimental observations, and the hidden ones, that must be estimated from experimental data by model inversion. For the observed parameters, we may need to set the level of accuracy of the experimental data and for those that mostly contribute to outputs' variabilities, more attention should be paid. Regarding hidden parameters, there is also a proper balance to find between the number of parameters used to describe the biophysical processes and the complexity of their estimation, which is always a bottleneck. By sensitivity analysis, we can rank the parameters by their significances to the system, or we can separate the parameters into different groups according to the interactions between the factors found by the sensitivity analysis. Then when we compute the estimation, according to the SA results, we can fix the least influential parameters, and we should pay more attention to those who play important roles in the outputs' variances.

In both cases, the sensitivity analysis may help to optimize the trade-off between experimental cost and accuracy. This is of crucial importance in the objective of developing a predictive capacity that scales from genotype to phenotype with the GreenLab model [8].

This paper is organized as follows: In section 2, we present a general overview of the sensitivity analysis methods and what could be their insights regarding the specific issues raised by the GreenLab model. In section 3, we apply the methods to the GreenLab model for maize and analyze the result. In section 4, we summarize and discuss the methodology, as well as its perspective.

2. Sensitivity Analysis: an overview

2.1. Characteristics of SA method

A model is represented by a mapping f (a deterministic or stochastic function) which relates the inputs domain to the output space:

$$Y = f(X_1, X_2, ..., X_k) \tag{1}$$

The input factors $(X_1, X_2, ..., X_k)$ are supposed to be random variables described by identified probability distributions which reflect the uncertain knowledge of the system under analysis. Y is taken to be a scalar, i.e. even in the application we shall consider each output variable in turn [2]. In the analysis application of plant growth next in section 3, we consider the biomass for each kind of organ at one certain growth cycle as one output. So when the time goes, the output varies in turn, then we get one set of result for the analysis.

2.2. Brief overview of the available methods

The most common classifications of available SA methodologies distinguish between quantitative and qualitative methods and between local and global techniques.

Qualitative methods are aimed at screening, while quantitative techniques can be designed to give information on the amount of variance explained by each factor. In general, the choice of which kind of method to use is driven by cost, as local or qualitative methods are computationally less expensive [9].

In local approaches (also known as one-at-a-time, OAT), the effect of the variation of a single factor is estimated by keeping all the others fixed at their nominal values. Yet they cannot include the effect of the shape of the density functions of the inputs, and they are not model independent.

Global approaches estimate the effect on the output of a factor when all the others are varying, enabling the identification of interactions in non-linear and/or non-additive models. Generally, global approaches allow the use of model independent methods as they do not require assumptions of additivity or linearity. As a drawback, they are usually computationally expensive to estimate [5].

The simplest and most intuitive way to obtain a local sensitivity index is to compute derivatives (see [10], [11], [12]). The sensitivity of the output Y to a perturbation of an input factor X_i is estimated at a given value X_i^*, as

$$Y'_{X_i} = \frac{\partial Y}{\partial X_i}\Big|_{x_i = x_i^*} \tag{2}$$

In situations where Y and X_i have different range of uncertainty, a more balanced measure can be obtained normalizing the derivatives by the factors' standard deviations:

$$S^{\sigma}_{X_i} = \frac{\sigma X_i}{\sigma Y}\frac{\partial Y}{\partial X_i}\Big|_{x_i = x_i^*} \tag{3}$$

The estimation of these OAT methods can be easily implemented, but they are informative only if the model is linear/Quasi linear or if the range of uncertainty of the input factors is small [5].

The Standardized Regression Coefficients (SRCs) can be viewed as the trade off between the local method and global method, concerning the advantages and shortcomings of the two: the accuracy of the analysis and the computing cost. It is based on the linear approximation of the model and Monte Carlo simulation. SRC method can demonstrate the shape of the probability distribution of every factor. The other important index produced by SRC is the model coefficient of determination, R^2, which represents the fraction of the output variance explained by the regression model itself. In the condition of $R^2 = 1$, the system is linear and the SRCs can totally explain the variance of the output affected by each factor. Even when models are moderately non-linear (i.e.$R^2 > 0.9$), the SRCs index can still be valid from a qualitative way. It will only explain 90% of the model's variance. When R^2 gets small, then the SRCs could not be reliable sensitivity presentation.

The other important category of SA method is called 'Variance based' method. The basic concept for this kind of method is to decompose the output variance into the contributions imputable to each input factor. The most widely used ones are the FAST (Fourier Amplitude Sensitivity Test, see [13], [14], [15]), and Sobol's method, see [16]. FAST method decomposes the output variance $V(Y)$ by means of spectral analysis. Sobol's method bases on the same decomposition of variance, which is achieved by Monte Carlo methods in place of spectral analysis. What we used in this paper is Sobol's method.

2.3. Common Steps of all SA Methods

Here we give the readers the general steps of SA and specify them in our application to Greenlab model.

2.3.1. Specify the target function of interest. It is easier to communicate the results of a sensitivity analysis when the target of interest has a direct relation to the problem tackled by the model. So to define the form of the output function that answers our questions would be the first thing before we do SA. In our analysis, the biomass generation and distribution of each kind of organ is the output we are interested in.

2.3.2. Assign a Probability Density Function (pdf) to the selected factors. When this involves eliciting experts' opinion this is the most expensive and time consuming part of the analysis as it may concerning long-time experiment. Especially for the plant growth model, huge amount of practice is needed to get the pdfs of the parameters. Though at the beginning of modeling, the structure of the model is needed to be set for the experiment, the pdfs of the factors can also be derived from the experiential knowledge, which can to some sense reflect the natural regulation. Or we can consider the pdfs as one reasonable hypothesis that might be one of the uncertainties of the modeling, which we will take into account when we do the SA afterwards to see how much this hypothesis has affected the result. What we adopted here is uniform distribution for all the parameters.

2.3.3. Generate a matrix of inputs with that distribution(s) through an appropriate design. As in experimental design, a good design for numerical experiments should give a maximum of effects with a minimum of computed points. In our analysis in the environment of C++, we use the 'Mersenne Twister random number generator' to get the sampling of the input data according to their pdfs.

2.3.4. Evaluate the model and compute the distribution of the target function. This is the computer-time intensive step. The major index of the output (the mean value and the variance) is computed by Monte Carlo Method.

2.3.5. Select a method for assessing the influence or relative importance of each input factor on the target function. The factors affect the choosing of the method for SA concern many aspect: the purpose of the analysis, e.g. model simplification, factor prioritizing, uncertainty reduction, etc; the characteristic of the model: linear, non-linear, quassi-linear, additive, etc; the computing cost the practitioner can afford...In [5], the author has given out a good sketch of the various techniques available and their use as a function of computational cost of the model and dimensionality of the input space.

3. Case study for plant growth model

3.1. Model description

GreenLab is a functional-structural model that simulates plant development, growth and morphological plasticity. The model simulates individual organ production and expansion as a function of the growth cycle (GC), which corresponds to the phyllochron (thermal time in degree days between the appearances of two consecutive leaves on the main stem) before the end of plant organogenesis for maize [17].

Plant organogenesis is controlled by GC and plant morphogenesis depends on biomass production and allocation to expanding organs or competing sinks. Biomass production per plant is thus simplified according to the following mathematical equation:

$$q^t(i) = E(i) \cdot \mu \cdot Sp \cdot [1 - exp(-\frac{\lambda}{Sp} \sum_{l=1}^{n(i)} S_l)] \qquad (4)$$

where $E(i)$ is an environmental function at growth cycle i (generally related to the Photosynthetically Active Radiation), μ is a conversion efficiency, λ is analogous to the extinction coefficient of Beer-Lambert's Law, S_p is a characteristic surface, $\sum S_l$ is photosynthetic surface areas of all leaves. Here λ is set to 0.7.

Organs receive an incremental allocation of biomass that is proportional to their relative sink strengths. The relative sink strength for each type of organ is defined as a function of its age in terms of GCs:

$$p_o(j) = P_o f_o(j) \qquad (5)$$

where o denotes organ type (b: leaf blade; s: sheath; e: internode; f: cob; m: tassel). P_o is the sink strength associated to organ type o. For leaf blade, $P_b = 1$ is set as a normalized reference. The relative sink strength for the first six short internodes is $K_e P_e$, with K_e an empirical coefficient. $f_o(j)$ is an organ type-specific function of sink variation. A normalization constraint

$$\sum_{j=1}^{T_o} f_o(j) = 1 \qquad (5A)$$

is set, with T_o being the maximum expansion duration for organ o that depends on the organ position.

In the course of organ development, its relative sink strength is assumed to vary according to a beta function f_o given by:

$$\begin{aligned} f_o(j) &= \begin{cases} g_o(j)/M_o & (1 \le j \le T_o) \\ 0 & (j \ge T_o) \end{cases} \\ g_o(j) &= (j + 0.5)^{\alpha_o} (T_o - j - 0.5)^{\beta_o} \\ M_o &= \sum_{j=1}^{T_o} g_o(j) \end{aligned} \qquad (6)$$

The parameters α_o and β_o vary with organ type. This function is flexible to describe the shape of the sink variation and can be fitted to data by optimization. Only one parameter (B_o) was optimized to define the beta function for each organ type, and the values of two parameters α_o and β_o in eqn.(6) are subsequently derived from B_o using the constraints $\alpha_o + \beta_o = 5$ and $B_o = [\alpha_o/(\alpha_o + \beta_o)]$.

At a given $GC(i)$, $d^t(i)$ is the demand of all expanding

organs :

$$d^t(i) = \sum_{o=b,s,e} P_o \cdot \sum_{j=1}^{i} f_o(j) + \sum_{o=f,m} P_o \cdot \sum_{j=1}^{i-1} f_o(j) \quad (7)$$

Therefore, the instantaneous value of biomass got by each kind of organ at $GC(i)$ is:

$$q_o^t(i) = \sum_{k=max(0,i-T_{ext})}^{min(T_o-1,i)} p_o(k) \frac{q^t(i)}{d^t(i)} \quad (8)$$

where T_{ext} stands for the GC at which organogenesis ceases for the whole plant. Note that for cob, the demand for biomass $p_f(k)$ is 0 before $15th$GC, and tassel only exists for two GCs: the $21th$ and $22th$. And the total time for the whole plant to be alive is 33GCs.

What we are also interested in is the accumulated biomass value for each kind of organ, which is just to add the instantaneous value of the organs' corresponding GC, and we use the capital letter Q to denote this class of values, in order to distinguish them with the instantaneous ones:

$$Q_o^t(i) = \sum_{n=0}^{i} q_o(n) \quad (9)$$

Note that there is the similar exception for cob and tassel as mentioned above.

We assume each uncertain input parameter has a uniform distribution which relies on the empirical knowledge, and we use the data from [7], [17], [18] to set the mean value and variance of all the parameters, which are listed in Table.1.

Table 1. Distribution characteristics for uncertain parameters

Parameters	Mean value	Variance
P_s	0.93	0.0537
P_e	1.63	0.0941
P_f	162.18	9.3635
P_m	1.33	0.0768
B_b	0.53	0.0306
B_s	0.7	0.0404
B_e	0.88	0.0508
B_f	0.58	0.0335
Sp	0.23	0.0133
μ	0.0046	0.0003

3.2. Local sensitivity analysis and its normalized version

The time evolution of $q_o^t(i)$ for the mean values of uncertain input factors is given in Fig.1.

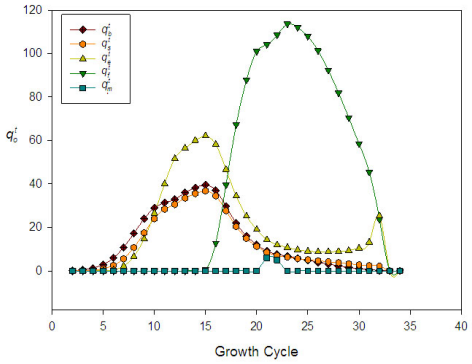

Figure 1. Biomass distributed to different organs at each GC

We took $q^t(i)$ for example to do the local sensitivity analysis and its normalized version presented in eqn.(2) and eqn.(3) respectively, the result is showed in Fig.2.

We used numerical simulation to get the derivatives of output $q^t(i)$. There are two ways to compute the standard deviations σY: the first one is Monte Carlo simulation, which we used and can be more reliable to calibrate the stochastic characteristics of the output variances but with heavy computing cost. To avoid this shortcoming, the other possibility is to use the following approximation:

$$(\sigma Y)^2 \cong \sum_i (\sigma X_i)^2 \left(\frac{\partial Y}{\partial X_i} \right)^2 \quad (10)$$

Such an approximation is justified when the system is highly linear, which we will evaluate in the following section.

For Fig.2, the sensitivity is better calibrated by the normalized version, because we took into account the differences in the ranges of variations of all the uncertain input factors. As for Sp, we can not even pick it out from other factors in the pure local analysis, but with the normalized one, the great contribution from Sp is better demonstrated from about $12th$ GC to the end of the plant's growth. And the basic knowledge we got from this local analysis is that the factor μ contributes the most to the variance of biomass generation from the beginning to the end.

Note that the point at which we calculate the derivatives is important, it could be not reliable for the system which has the parameter-to-output curve with many apices, then the derivative will be either too big or too small, and the value at these special points can not stand for the whole character of sensitivity for this parameter. In this case, the result could be misleading, and we may miss the important details of the system. So we will introduce applications of other methods next.

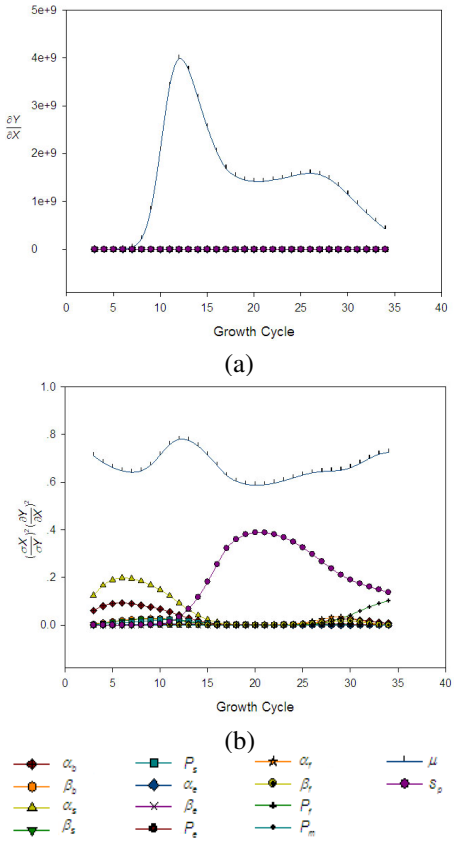

Figure 2. a. Pure local sensitivity of q^t with respect to the factors listed in table.1, absolute value. b. Normalized local sensitivity of q^t with respect to the factors listed in table.1, absolute value. Y in the vertical axes label indicates q^t, X in the vertical axes label indicates the parameters, depending on the curves.

3.3. Standardized Regression coefficients

To check whether the growth model for maize is linear in its input factors corresponding to the output we are interested in, the Standardized Regression coefficients (SRCs) can be used (see section 2.2). Indicating with the parameters listed in table.1 as X_i, still with q^t, q_o^t, Q^t, Q_o^t the output variables as Y respectively, the following regressions are fit:

$$Y = b_0 + \sum_i b_{X_i} X_i \tag{11}$$

To change this dimensioned coefficients values to the standardized ones, the following comes the SRCs:

$$\gamma_{X_i} = \frac{\sigma X_i}{\sigma Y} b_{X_i} \tag{12}$$

Note that if the factors are independent and the true model (for example, the plant growth model for maize) is linear, then the following equation is hold (see [19]):

$$\sum_i (\gamma_{X_i})^2 = 1 \tag{13}$$

The sum of $(\gamma_{X_i})^2$ is therefore can be considered as a index of the model linearity. This sum is described also by the called 'model coefficient of determination', which is computed as:

$$R_Y^2 = \sum_{d=1}^{N} \frac{(Y^* - \mu_Y)^2}{(Y - \mu_Y)^2} \tag{14}$$

where μ_Y is the mean value of Y in the Monte Carlo simulation (200000 runs for our simulation), Y^* is the fitted value in eqn.(11), Y is the actual value in each run, and N is the total number of runs.

Still we take the result with output q^t as example, which is shown in Fig.3. Note that the SRCs result is similar to the squared normalized local measures, which is not a coincidence, for the linear system, the two should be equal to each other. To affirm this linearity conclusion, the two methods of linearity computing are showed in Fig.4.

Both of the linearity indexes show that even lower at the beginning and drop twice from around $5th$ to $15th$ GC, the whole linearity of the system is high (all above 0.94) when the output of q^t is considered. So the result of SRCs and squared normalized local measures tend to be equal in our case. For there is not uniform standard to say the system could be considered linear when the linearity index is above one certain value for different systems (in [5], the standard is set at 0.8), especially for the result in Fig.4 with waves. So to be cautious, we consider the smooth part which maintain a relatively higher value as linear in our simplification, for maize, it is from $21th$ GC to the end. In this way, the regression analysis could be used as a preliminary step in SA to save the computing cost before we really do some complicate analysis. And if the linearity index is low, for instance below 90%, we must find one appropriate global analysis result for the analysis, which we will present next.

3.4. Variance decomposition-based sensitivity measure: Sobol's method

The basic idea of Sobol's method (see [16]) is to decompose the function of eqn.(1) into terms of increasing dimensionality:

$$\begin{aligned} f(X_1, ..., X_k) &= f_0 + \sum_{i=1}^{k} f_i(X_i) \\ &+ \sum_{1 \le i < l \le k} f_{il}(X_i, X_l) \\ &+ \cdots + f_{1,2,...,k}(X_1, ..., X_k) \end{aligned} \tag{15}$$

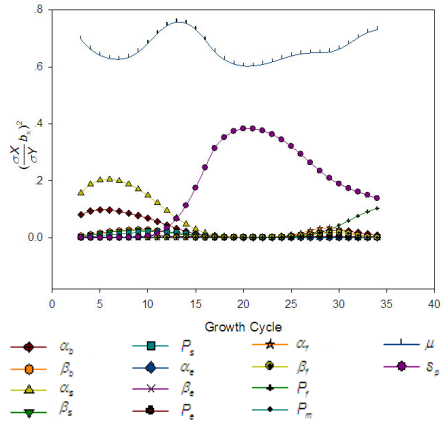

Figure 3. The SRCs for output of q^t. The vertical axes denotes for the SRCs depending on the curves explaining different parameters.

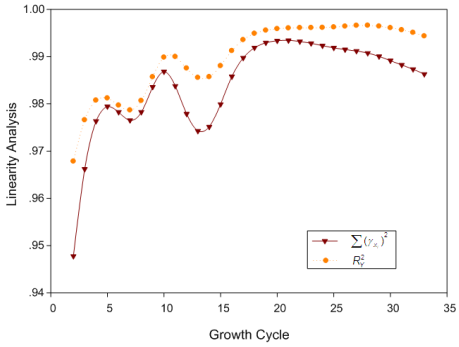

Figure 4. $\sum(\gamma_{X_i})^2$ and R_Y^2 for output of q^t

If the input factors are mutually independent then there exists a unique decomposition of eqn.(15), such that all the summands are mutually orthogonal. The variance of the output variable Y can be therefore decomposed into:

$$V(Y) = \sum_{i=1}^{k} V_i + \sum_{1\le i<l\le k} V_{il} + \cdots + V_{1,2,\ldots,k} \qquad (16)$$

Where V_i, V_{il}, $V_{1,2,\ldots,k}$ denote the variance of f_i, f_{il}, $f_{1,2,\ldots,k}$ respectively. In this approach the first-order sensitivity index for factor X_i defined in eqn.(1) is given by:

$$S_i = \frac{V(E(Y|X_i))}{V(Y)} = \frac{V_i(E_{-i}(Y|X_i))}{V(Y)} \qquad (17)$$

where E and V indicate, respectively, the mean an variance operators and $-i$ indicate all factors but i. The inner expectation is taken at a generic point in the space of variable X_i, while the outer variance is over all possible values of this generic point.

The higher order sensitivity indexes $S_{i_1,\ldots,i_s}$ are given by:

$$S_{i_1,\ldots,i_s} = \frac{V_{i_1,\ldots,i_s}}{V(Y)}$$

for $s > 1$, eqn.(16) can be rewritten in terms of sensitivity indexes as:

$$1 = \sum_{i=1}^{k} S_i + \sum_{1\le i<l\le k} S_{il} + \cdots + S_{1,2,\ldots,k} \qquad (18)$$

In [20], a computationally efficient design is discussed, which we used in our simulation processing.

As the result we got here with the same parameter space as in section 3.2 and section 3.3 with output q^t is similar to the two for the high linearity of the system we mentioned in section 3.3. And we have already known that the parameters Sp and μ take as high as $75\%\sim98\%$ of the summation for first-order index and the whole first-order sensitivity index contribute to $93\%\sim99\%$ of the systems' variance in the former analysis. So as one alternative parameter space, we fixed Sp and μ at their mean value, and applied Sobol's method again, to our expectation, since the majority part of the uncertainty is excluded by us and the detailed sensitivity of the other uncertainty input should be clearer. And the result proved our deducing. The other important conclusion is that after we fixed the two most sensitive parameters, the system becomes less linear. Fig.5 and Fig.6 are showed to demonstrate these points.

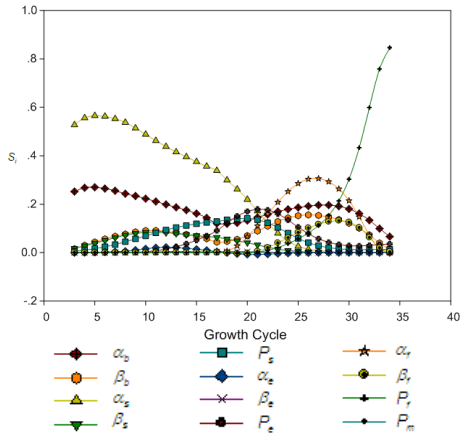

Figure 5. Sobol's method for SA with parameter space of Sp and μ fixed

Note that without Sp and μ, α_s and α_b play the most important role in the system at the first 21 GCs, and after which α_f takes the role instead, but with less amount than α_s, until the $30th$ GC, the sensitivity of P_f rises dramatically while all the other parameters dropping. This trend can be explained in the botany world: at the beginning of the maize's growth, before the fruit appears, the factors that control the competition of biomass acquisition must play an important role, here they are α_s and α_b for internodes' and blades' growth. Afterwards, the fruit (cob) starts appearing, then most of the biomass produced goes to the fruit, during which α_f has a strong influence. But its value is generally

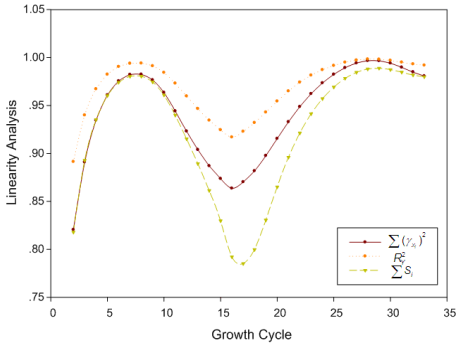

Figure 6. The three kinds of linearity indexes with parameter space of Sp and μ fixed

not as high as α_s, because in this time period, the other organs still play relatively important roles. The biomass absorbed by the fruit is mainly produced by the blades and simultaneously, new blades and internodes still keep appearing while some of the old ones keep expanding and some die. So the whole variance of the system output tends to be shared more uniformly during this stage between most parameters. After the $31th$ GC, all other organs stop growing except the cobs, which still accumulate biomass, and the sensitivity coefficient of P_f increases dramatically.

In Fig.6, we show the two indexes which give the linearity level of the system, along with the summation of all S_i. We noticed that the trends which they express agree to each other. So the summation of S_i also has the characteristic of linearity index. Actually it can be explained from the definition of S_i: the more the sum of the first-order indexes is close to 1 in eqn.(18), the more mutually independent the factors are, and the more linear the system is. In the new parameter space without Sp and μ, the system linearity is weaker, especially from $10th$ GC to $23th$ GC, which is the most non-linear stage of the growth, corresponding to abrupt changes in the allocation dynamics due to cob appearance.

4. Discussion

As in GreenLab model we need valid tools to locate the sources of uncertainty and evaluate them in a quantitive way. Sensitivity analysis is an efficient tool for this purpose and was used to assess the significance of GreenLab model parameters, based on the methods described in [5], [9].

For the simple ranking of the whole pack of parameters, we can get that the most important parameters for plant growth model of maize are μ and Sp, which can take responsible for almost $75\%\sim98\%$ of the first-order sensitivity index. *Coefficient of sink strength P_o generally does not contribute so much to the system's variance, except for P_f at the last 2 GCs of the growth, which means in the parameter estimation for modeling afterward, we can fix this group of parameters to simplify the computing.*

If we fix the most important factors that we have already found, we can get the detailed sensitivity characters of the other factors, but notice that this kind of method relies on the fact that the second order sensitivity coefficients of the other parameters to the ones fixed should be relatively small, which means the co-relationship between the fixed factors and the kept variables should be slim, so that the disappearance of the variance for the most important ones will not imply missing the corresponding second order intercourse variances. In our case, this condition is confirmed by the linearity analysis of the system. Linearity analysis can also be used to choose the best SA method, with proper computing cost.

Though the distribution of the parameters is hard to get, if the experiment allows, we can get a much more specified analysis result when the distribution information can be as plentiful as possible. In fact, we have tried both Gaussian and uniform distribution for the parameters in our analysis, the results do not get so much different. Maybe it just needs an approximate range that is easier for us to get from the experiment than to get the accurate distribution of the parameters, see [21] and [22] for the sampling method and proper method to get experimental data for this analysis.

In future works, we should account for the interactions with the environmental factors, then to assess the most important environment factors at different growth stage, according to the stress levels. As for this, the method we use should be changed for large scale sensitivity analysis, see [23], [24], [25], in which the most popular method is Morris's [26].

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